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Electronic band structure of a Carbon nanotube superlattice

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ABSTRACT

By employing the theoretical method based on tight-binding, we study electronic band structure of single-wall carbon nanotube (CNT) superlattices, which the system is the made of the junction between the zigzag and armchair carbon nanotubes. Exactly at the place of connection, it is appeared the pentagon–heptagon pairs as topological defect in carbon hexagonal network. The calculations are based on the tight binding model in the nearest-neighbor approximation. We seek to describe electronic band structure in the presence of the pentagon-heptagon pairs. Our calculation show that the pentagon–heptagon pairs defect in the nanotube structures is not only responsible for a change in a nanotube diameter, but also governs the electronic behaviour around Fermi level. Also, we obtain the Fermi energy of the system via integration of the density of states and matching it to the number of electron in the unit cell. The numerical results may be useful to design of electronic devices based on CNTs.

Keywords: *Carbon nanotube; Tight–binding model; Pentagon-heptagon pair defect; Band structure; SW defect.*

INTRODUCTION

Carbon nanotubes (CNTs) are quasi-one-dimensional nanostructures with unique electrical properties that make them ideal candidates for applications in nanoelectronics. Since the discovery of carbon nanotubes (CNTs) just over a decade ago [1], their unique electronic and structural properties have aroused great excitement in the scientific community and promise a broad range of applications. A wide variety of nanotube-based electronic devices, such as diodes, transistors, or field emitters [2-4], has been already theoretically modeled and experimentally achieved. The studies show that the CNT can be metallic or semiconducting depending on diameter and chirality [5, 6]. By joining two perfect CNTs one can form a superlattice by introducing pentagon–heptagon pairs at the interface [5]. Following this idea, a number of CNT superlattices [7, 8], junctions [9], and nanodevices [10] have thus been obtained.

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In the case of the topological defects into the hexagonal carbon network, the nanotube chirality may change and therefore its electronic characteristics. In our recent work, we have introduced a simple method to investigate electronic transport in quasi one dimensional systems (such as the pure and superlattice like disordered carbon nanotubes) by mapping of its real-space to one-dimensional mode space [11]. In the mentioned system, the disorder is uniformly distributed in direction of the nanotube axis. In this paper, we investigate the electronic band structure of a typical superlattice $n(12, 0)/n(6, 6)$ on base of tight binding model. Then, we represent the calculations and results for the electronic band structure for these systems [12-14].

The paper is organized as follows: At first, the calculation model is explained after introduction. Then, the obtained numerical results of this work are discussed. The paper is concluded in the last section.

EXPERIMENTAL

Computational methods

We have performed the electronic structure calculation on the base of tight-binding model within the nearest-neighbor π-electron approximation. The second-neighbor interactions are neglected. In this work, a unit cell of CNT zigzag joined to an armchair (exactly at the place of connection) appears a pentagon–heptagon pair topological defect [15-18] in carbon hexagonal network. These defects form quantum wells/barriers for the electron waves in the system. They can be created by local rotating of a C–C bond by 90° resulting in two pentagons connected by a pair of heptagons, without changing the overall helicity of the tube and the number of the atoms (vertexes) does not change [19]. The rotation only affects four adjacent hexagons, converting two into pentagons and two into seven-sided heptagons. This particular 5-7-7-5 configuration has been studied extensively and is known in the literature as a Stone-Wales (SW) defect [20]. In a semiconducting CNT, the energy gap or the density of states at the Fermi level are determined by the density of SW defects [21]. SW defects can reduce the band gap and close it in the large band gap CNTs and increase the density of states in the metallic CNTs [19].

As one can see from Figure 1, two subslices create the unit cell of superlattice with thickness of d. For simplicity, we have applied the hoping energy and onsite energies in each supercell and also interaction of supercell with each other. In our calculation, the hopping parameter is fixed to $t = -2.7$ eV. The unit cell of superlattice contains a unit cell (12, 0) with another unit cell (6, 6). Thus, for 1(12, 0)/1(6, 6) system, there are 72 atoms in the unit cell. These are grouped in 6 atomic layers. Also, they are introduced six pentagon-heptagon pairs (the SW defects) at their interface (see the Figure 1). To change the concentration of SW defect in a CNT and to investigate the effect of defect–defect interaction on the defect formation energy, the size of the supercell containing a SW defect is increased. Moreover, we have calculated other type of systems: 2(12, 0)/2(6, 6), 3(12, 0)/3(6, 6) and 4(12, 0)/4(6, 6), which have 144, 216 and 288 atoms in supercells, respectively.

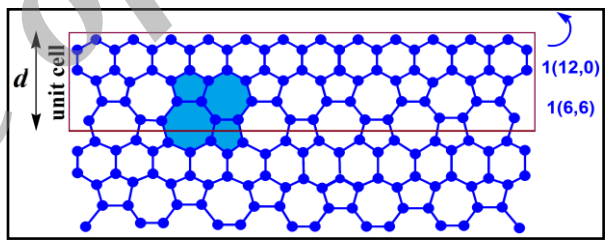

Fig. 1. Schematic representation of the carbon nanotubes junction composed one slice zigzag (12, 0) contacts to one slice armchair (6, 6) via the pentagon–heptagon pairs as topological defect in carbon hexagonal network. The rolling of the nanotube is indicated by arrow. The lengh of unit cell in the superlattice is d.

RESULTS AND DISCUSSION

At first, we have plotted the electronic band structure of the single-walled (12, 0) and (6, 6) carbon nanotubes as shown in Figure 2 (a) and (b), respectively. These kinds of CNT are always metallic without a band gap, which they are the k-points in the Fermi level at zero energy. Here, the length of unit cell is chosen as 4.26 Å and 1.42 Å, respectively. The results obtained for energy dispersion can be concerned with a good approximation for the purpose of understanding electron transport properties.

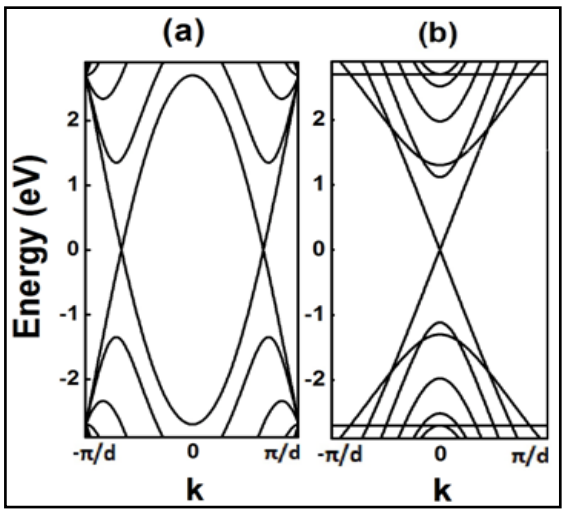

Fig. 2. The subband structures of single-walled (a) armchair tube (6,6) and (b) zigzag tube (12,0), which the lenghs of unit cell are d=1.42 Å and d=4.26 Å, respectively. Fermi level is at zero energy.

In order to understand the electronic properties of CNT superlattice, we have calculated electronic band structure of the junction between the zigzag and armchair CNTs (n(12, 0)/n(6, 6) system for n = 1, 2, 3 and 4). In all calculation, the hopping parameter in the defect region is also considered before. The results for 1(12, 0)/1(6, 6), 3(12, 0)/3(6, 6) and 4(12, 0)/4(6, 6) CNT superlattices have been plotted in Figure 3 (a)-(d). In all panels the dotted line shows the Fermi energy of the superlattice structure. The Fermi level crosses energy bands at 0.05 eV, 0.44 eV and 1.19 eV, respectively. The reason for this is related to appearance of pentagon–heptagon pairs at junction region as a topological defect. This effect leads to break the electron-hole symmetry, and therefore the Fermi level for the system shifts to top and bottom of zero energy. The results show that the SW defects affect the conductance of metallic CNTs and generate quasibond states and exhibit quantized conductance reduction [22]. We can see that the electronic band gap appears in 2(12, 0)/2(6, 6) CNT superlattice, that is, this system is semiconducting (the Fermi level set on -0.07 eV at the valence band edge). This can be interpreted in terms of extra charge carriers (holes) at the Fermi level and this system is a semiconductor p-type. The other cases, the structures are metallic. This effect is due to the existence of pentagon–heptagon interface effects, which break the electron-hole symmetry. Likewise with increasing atoms, the energy bands of the superlattices in the vicinity of the Fermi level become flat in from but the energy bands have more bend far from the Fermi level.

In one-dimensional metals, composed of chains of atoms or molecules, bond alternations occur which open up a band gap, a phenomenon known as Peierls distortion [23]. Similar treatment is seen for one-dimensional conducting polymers, which they are not metallic properties at room temperature without doping. Although metallic single-walled CNTs are one-dimensional metals, but the coupling between slices of different CNT (as known superlattice) lead to open a band gap (semiconducting). The reason for this is due to the pentagon–heptagon pairs as topological defect in carbon hexagonal network. That is, the interwoven carbon bonds can be easily distorted to open a band gap. Therefore, Peierls distortion may be expected in single-walled CNT superlattice.

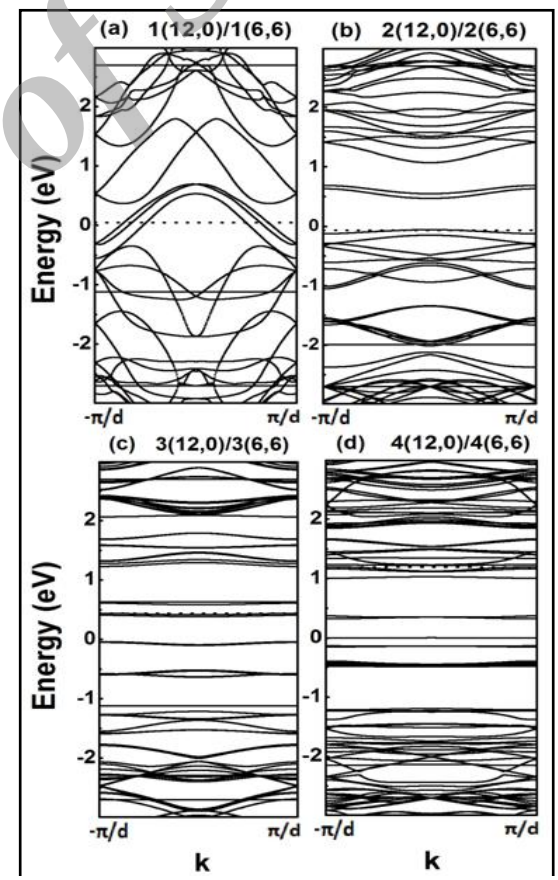

Fig. 3. Band structure of n(12,0)/n(6,6) superlattices around E_F for (a) n=1, (b) n=2, (c) n=3 and (d) n=4. The Fermi level for (a)-(d) are 0.05, -0.07, 0.44 and 1.19eV, respectively, which are shown by dashed line in all panels. The lengths of superlattice unit cell are 8.904 Å for n=1, 13.394 Å for n=2, 20.12 Å for n=3 and 26.838 Å for n=4. Each unit cell of the system has 72, 144, 216 and 288 atoms, respectively.

The main objective here is to use the idea of band-gap engineering to fabricate quantum well/barrier structures that have very narrower passbands for filter applications. Each substructure of the superlattice can produce its own band structure as discussed in previous section.

CONCLUSIONS

The electronic band structure of CNT superlatice for (12, 0)/1(6, 6), 2(12, 0)/2(6, 6), 3(12, 0)/3(11, 0) and 4(12, 0)/4(6, 6) have been studied dy the tight–binding model. We have shown that the pentagon-heptagon pairs appear as topological defects at junction in carbon hexagonal network. We have found for $n = 1, 2$ and 3, the Fermi level crosses energy bands Therefore these systems are metallic but for 2(12,0)/2(6,6) CNT superlattice, the Fermi level set on at the valence band edge and we see band gap between the valence and the conduction band then this system is semiconductor. This effect is due to the existence of pentagon–heptagon interface effects, which break the electron-hole symmetry.

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